

Rotational Spectroscopy in Support of Upper Atmospheric Research at JPL

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Rotational spectroscopy at JPL supports the NASA's Upper Atmospheric Research Program by providing a database of rotational transitions and by performing laboratory measurements to improve the database as required by the observational programs. Of prime concern are the spectroscopic needs of the EOS-MLS (Earth Observing System – Microwave Limb Sounder) experiment. Because air-broadened linewidth measurements of rotational transitions are sparse, the JPL compilation of rotational spectra does not include any linewidth information. Several of the transitions that will be observed by EOS-MLS will require improved accuracy of their linewidth parameters. The MLS requirements will be presented and the laboratory program to satisfy the requirements will be described. Current measurements of the HCl $J = 1 - 0$ transition near 625.9 GHz will be used to illustrate the work in progress. These measurements will be compared to those of the corresponding transition in the vibrational spectrum and to measurements made in other laboratories.

Because of the role of the halogen oxides in upper atmospheric processes resulting in ozone depletion, our studies are also directed toward better determination of their molecular properties as well as their spectra. Recently we have extended the range of observations of ClO, BrO, and IO. In the process of these investigations, we discovered that we were able to generate IO and BrO in highly excited vibrational states, $v = 13$ in $X_1^2\Pi_{3/2}$ and $v = 9$ in $X_2^2\Pi_{1/2}$ for IO and $v = 8$ in $X_1^2\Pi_{3/2}$ and $v = 7$ in $X_2^2\Pi_{1/2}$ for BrO. In addition, we used ^{18}O enrichment to observe the isotopically-substituted molecules. For ClO the excitation mechanisms which were effective in the heavier oxides do not seem to occur. However, ClO is generated in high yield and we were able to observe $v = 2$ spectra at thermal populations and ^{18}O spectra in natural abundance. Isotopically independent parameters will be presented for ClO, BrO and IO and interpreted in terms of their interatomic potentials and electron distributions.

OIO was discovered as a byproduct of the IO reactions. These were the first high-resolution observations of OIO. As is the case for OClO and OBrO, OIO has a 2B_1 ground electronic state. Both the ground vibrational state and first excited bending state spectra of the X^2B_1 state have been analyzed. Thus, precise molecular parameters are now available for the series of compounds, OClO, OBrO and OIO. Their structures and electron distributions will be compared.

Related compounds for which spectra have been analyzed include ClOClO₂, ClClO₂, HOClO₃ (perchloric acid), and FClO. The status of the halogen oxide spectra included in the JPL database will be discussed.